

WE CLAIM:

1. A co-crystal comprising FimC, FimH and mannopyranoside in crystalline form.

5 2. The co-crystal of Claim 1 in which the FimC or FimH is a mutant.

3. The co-crystal of Claim 2 in which the mutant is a conservative mutant.

4. The co-crystal of Claim 2 in which the FimH is FimH Q13 N

10 5. The co-crystal of Claim 2 in which the FimH comprises amino acids 1 to 158
of SEQ ID NO:4.

15 6. The co-crystal of Claim 1, which is diffraction quality.

7. The co-crystal of Claim 1, which is a native crystal.

8. The co-crystal of Claim 1, which is a heavy-atom derivative crystal.

20 9. The co-crystal of Claim 1, which is characterized by a unit cell of $a=138.077 \pm 0.2\text{\AA}$, $b=138.130 \pm 0.2\text{\AA}$, $c=215.352 \pm 0.2\text{\AA}$, $\alpha=90$, $\beta=90.005$, and $\gamma=90$.

10. The co-crystal of Claim 1, which is produced by a method comprising the steps
25 of:

(a) mixing a volume of a solution comprising FimC, FimH and mannopyranoside
with a volume of a reservoir solution comprising a precipitant; and

(b) incubating the mixture obtained in step (a) over the reservoir solution in a
closed container, under conditions suitable for crystallization until the crystal
forms.

30 11. The co-crystal of Claim 10, wherein the precipitant is present in a
concentration between 0.6 M and 1.2 M.

12. The co-crystal of Claim 10 wherein the precipitant is ammonium sulfate.

13. The co-crystal of Claim 10, wherein the solution further comprises between 50 mM and 100 mM Tris HCl.

14. The co-crystal of Claim 10, wherein the solution comprises between 0.5 mM and 30 mM mannopyranoside.

5 15. The co-crystal of Claim 10, wherein the solution has a pH of between 7.8 and 8.6.

10 16. A method of making the crystal of Claim 1, comprising:

- (a) mixing a volume of a solution comprising the FimC, FimH and mannopyranoside with a volume of a reservoir solution comprising a precipitant; and
- (b) incubating the mixture obtained in step (a) over the reservoir solution in a closed container, under conditions suitable for crystallization until the crystal forms.

15 17. The method of Claim 16, wherein the precipitant is present in a concentration between 0.6 M and 1.2 M.

20 18. The method of Claim 16, wherein the precipitant is ammonium sulfate.

19. The method of Claim 16, wherein the solution further comprises between 50 mM and 100 mM Tris HCl.

25 20. The method of Claim 16, wherein the solution comprises between 0.5 mM and 30 mM mannopyranoside.

21. The method of Claim 16, wherein the solution has a pH of between 7.8 and 8.6.

30 22. A machine-readable medium embedded with information that corresponds to a three-dimensional structural representation of a co-crystal comprising FimC, FimH, or a fragment or portion thereof, and a mannose sugar in crystalline form.

35 23. The machine readable medium of Claim 22, in which the crystal is diffraction quality.

24. The machine readable medium of Claim 22, in which the crystal is a native crystal.

5 25. The machine readable medium of Claim 22, in which the crystal is a heavy-atom derivative crystal.

10 26. The machine readable medium of Claim 22, in which the FimC or FimH is a mutant.

15 27. The machine readable medium of Claim 26, in which the mutant is a selenomethionine or selenocysteine mutant.

20 28. The machine readable medium of Claim 27, in which the mutant is a conservative mutant.

25 29. A machine-readable medium embedded with the atomic structure coordinates of Figure 2, or a subset thereof.

30 30. A method of identifying a FimC or FimH binding compound, comprising the step of using a three-dimensional structural representation of complex comprising FimC, FimH and mannopyranoside, or a fragment thereof, to computationally screen a candidate compound for an ability to bind FimC or FimH.

35 31. A method of identifying a FimC or FimH binding compound, comprising the step of using a three-dimensional structural representation of complex comprising FimC, FimH and mannopyranoside, or a fragment thereof, to computationally design a synthesizable candidate compound that binds FimC or FimH.

30 32. A machine-readable medium embedded with the atomic structure of Table 14 or Table 16, or a subset thereof.

35 33. A co-crystal comprising FimC, FimH ,and a saccharide.